Full wwPDB EM Validation Report ⓘ

Oct 28, 2026 – 12:12 pm GMT

PDB ID	:	9TG1 / pdb_00009tg1
EMDB ID	:	EMD-55887
Title	:	Structure of endogenous human ncBAF bound to nucleosome
Authors	:	Arias Pinto, C.; Guan, Y.; Concordet, J.P.; Ben-Shem, A.; Papai, G.
Deposited on	:	2025-11-28
Resolution	:	2.75 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

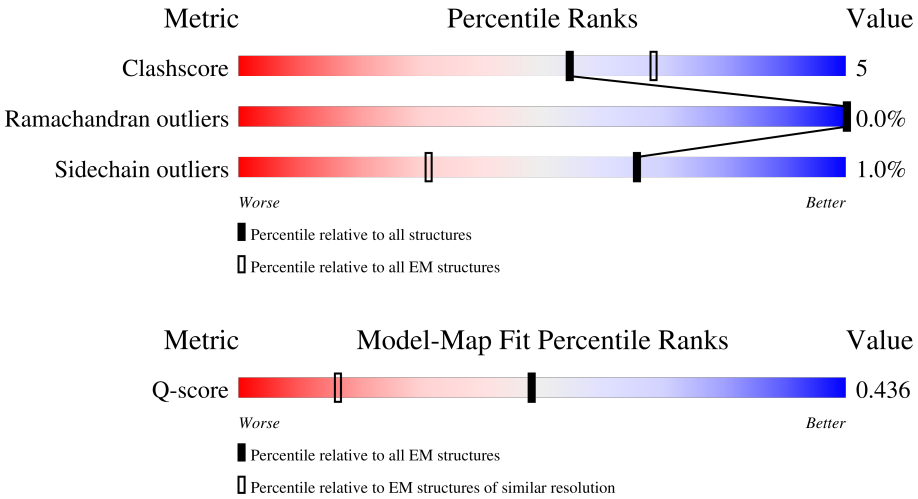
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	1647	36% 60%
2	A	136	70% 29%
2	E	136	59% 8% 29%
3	B	103	77% 19%

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Mol	Chain	Length	Quality of chain
3	F	103	66% 10% 24%
4	C	130	76% 21%
4	G	130	78% 19%
5	D	126	70% 6% 25%
5	H	126	71% 26%
6	I	131	57% 43%
7	J	131	67% 33%
8	L	597	17% 15% 5% 80%
9	O	210	5% 6% 94%
10	M	375	10% 80% 15%
11	N	429	75% 8% 17%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	657	Total	C	N	O	S	0	0
			5439	3456	979	976	28		

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	97	Total	C	N	O	S	0	0
			801	505	155	138	3		
2	E	97	Total	C	N	O	S	0	0
			800	503	155	139	3		

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
3	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 4 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	103	Total	C	N	O	0	0
			795	501	155	139		
4	G	105	Total	C	N	O	0	0
			809	510	158	141		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897

- Molecule 5 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
5	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 6 is a DNA chain called DNA (131-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	131	Total	C	N	O	P	0	0
			2669	1268	484	786	131		

- Molecule 7 is a DNA chain called DNA (131-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	131	Total	C	N	O	P	0	0
			2702	1279	506	786	131		

- Molecule 8 is a protein called Bromodomain-containing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	117	Total	C	N	O	S	3	0
			988	635	173	170	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	240	GLU	GLN	conflict	UNP Q9H8M2

- Molecule 9 is a protein called B-cell CLL/lymphoma 7 protein family member A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	13	Total	C	N	O	0	0
			65	39	13	13		

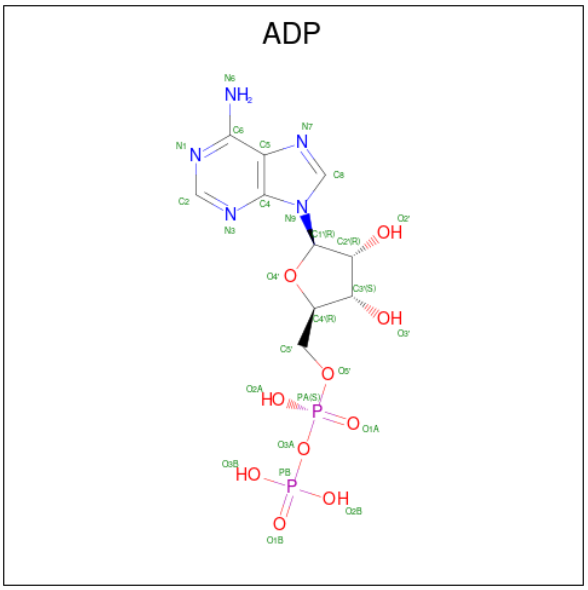
- Molecule 10 is a protein called Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	360	Total	C	N	O	S	0	0
			2821	1786	474	543	18		

- Molecule 11 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	356	Total	C	N	O	S	0	0
			2787	1767	470	529	21		

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

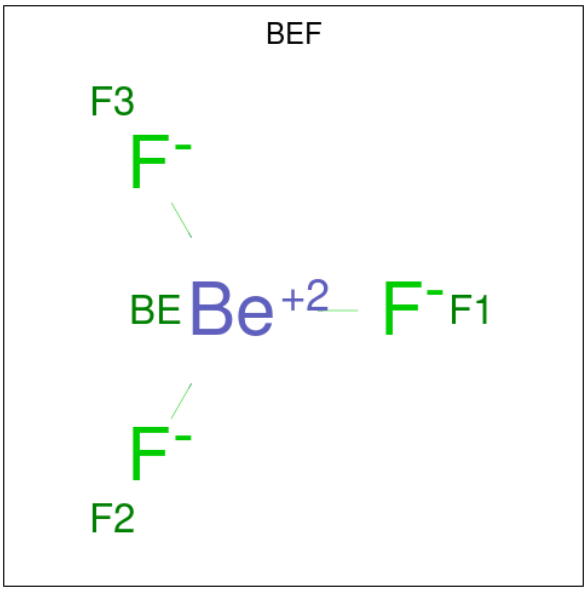


Mol	Chain	Residues	Atoms					AltConf
12	K	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Mg	0
			1	1	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
14	K	1	Total	Be	F	0
			4	1	3	

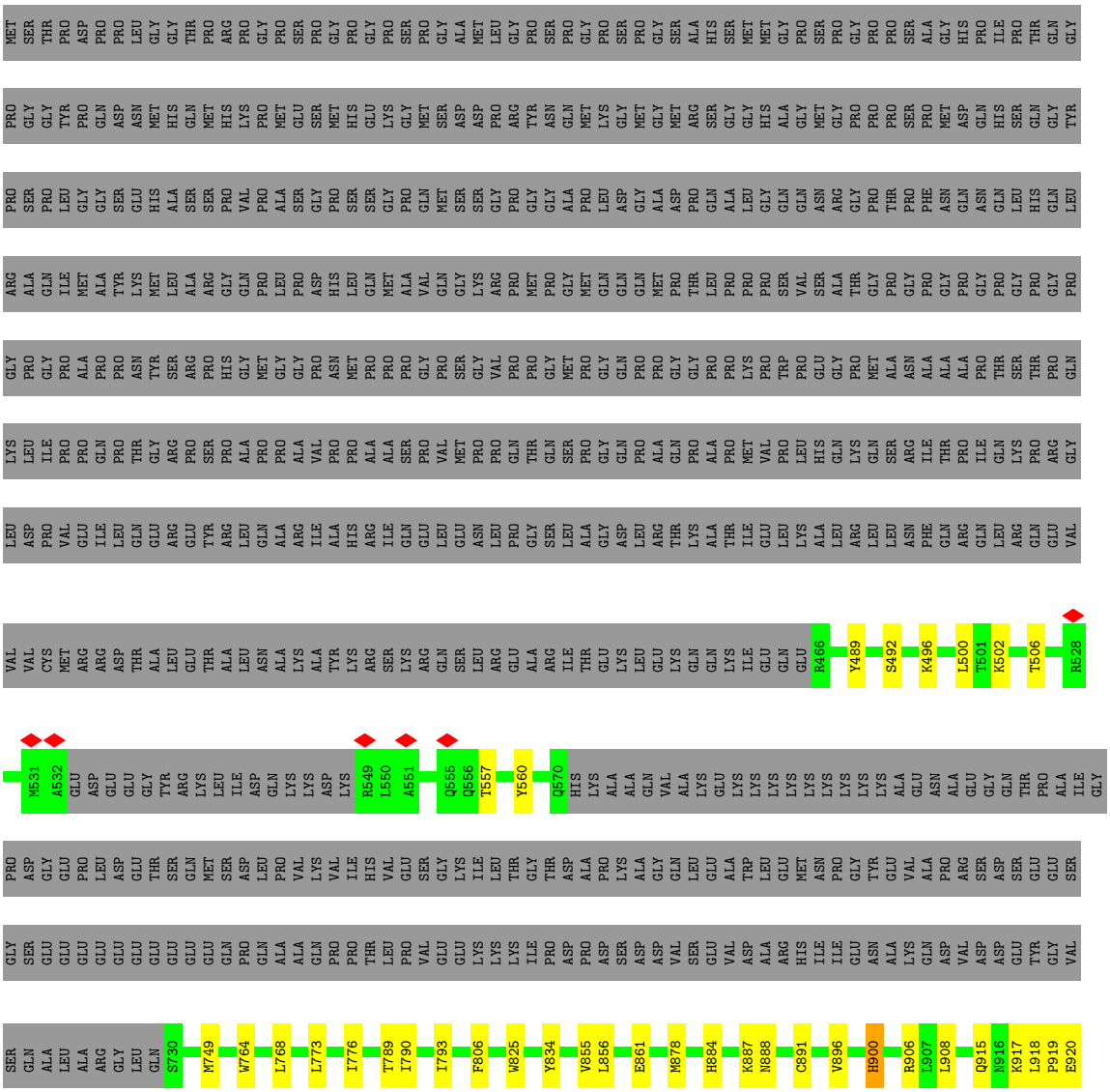
3 Residue-property plots (i)

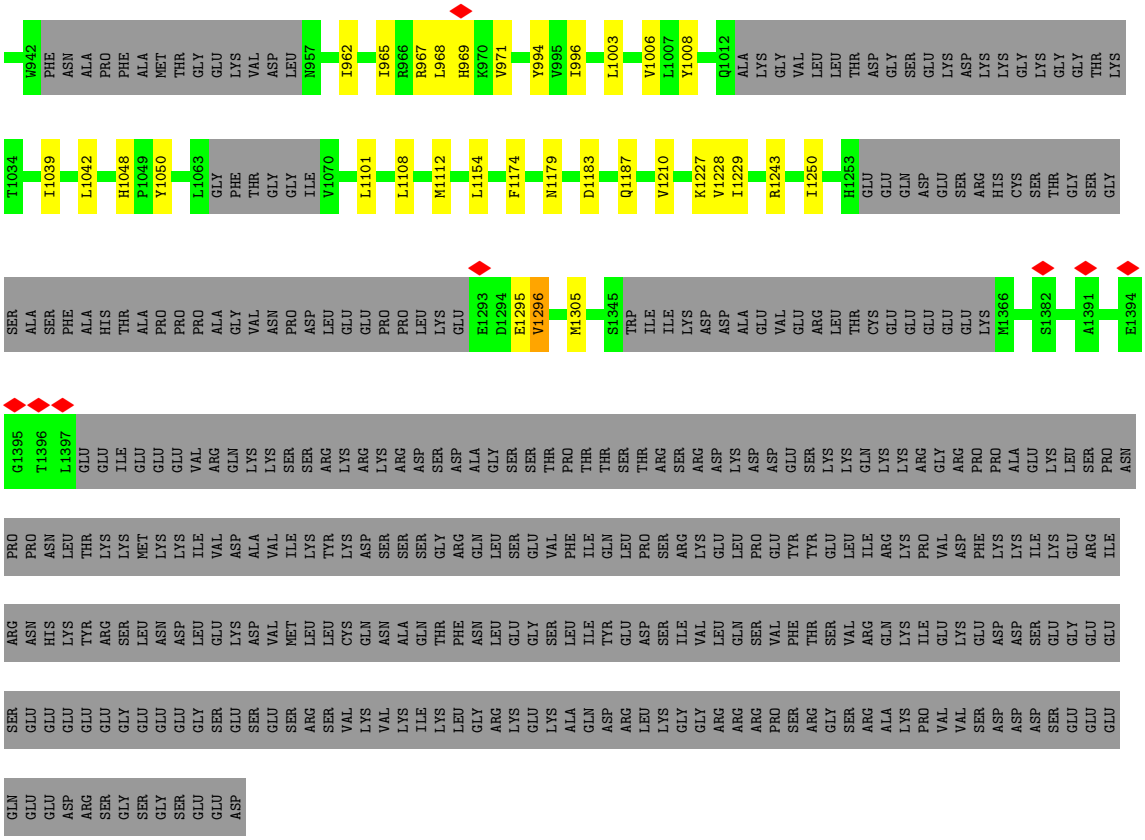
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transcription activator BRG1

Chain K:



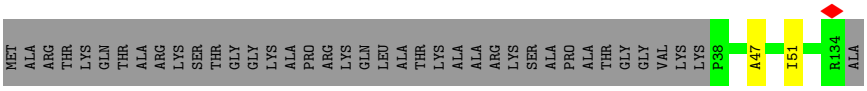




• Molecule 2: Histone H3.2

Chain A:

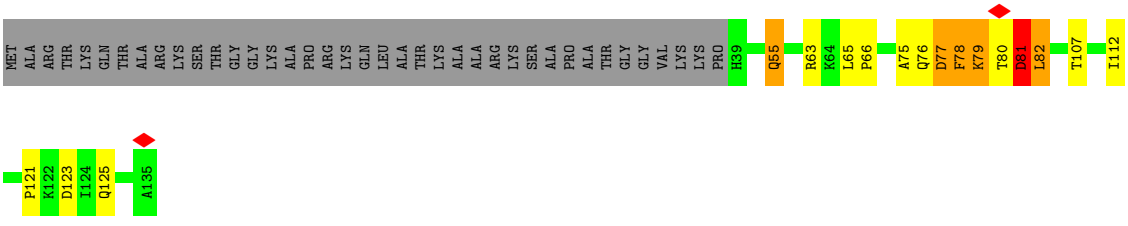




• Molecule 2: Histone H3.2

Chain E:

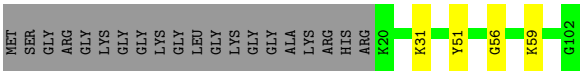




• Molecule 3: Histone H4

Chain B:

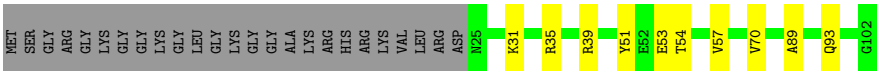




• Molecule 3: Histone H4

Chain F:

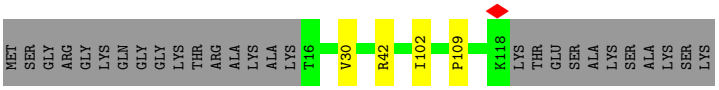




• Molecule 4: Histone H2A type 1

Chain C:

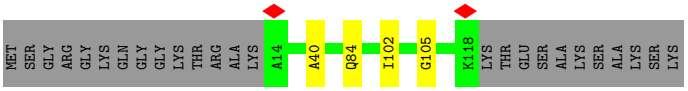




• Molecule 4: Histone H2A type 1

Chain G:

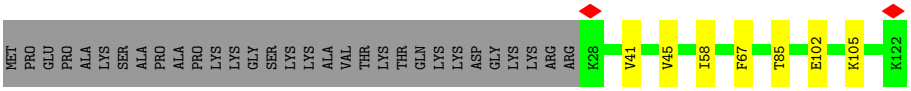




• Molecule 5: Histone H2B 1.1

Chain D:

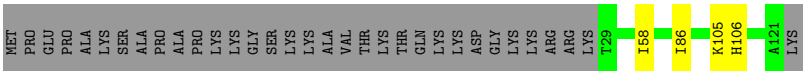




• Molecule 5: Histone H2B 1.1

Chain H:

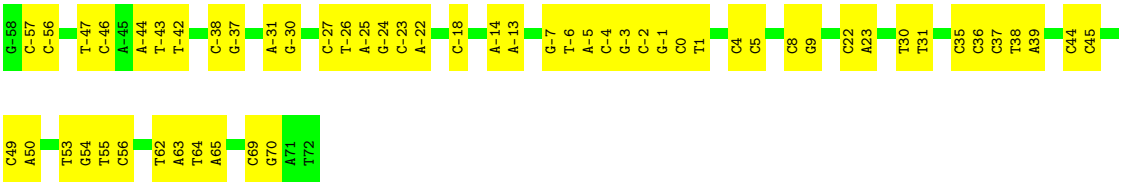




• Molecule 6: DNA (131-MER)

Chain I:

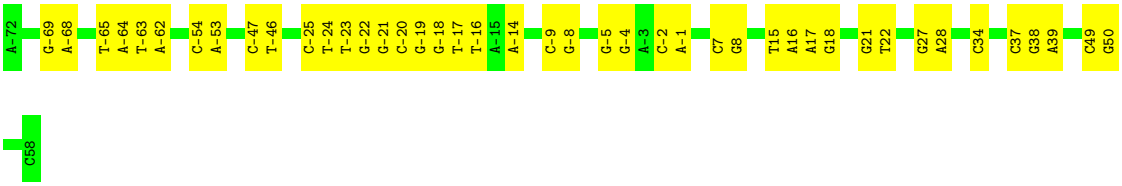




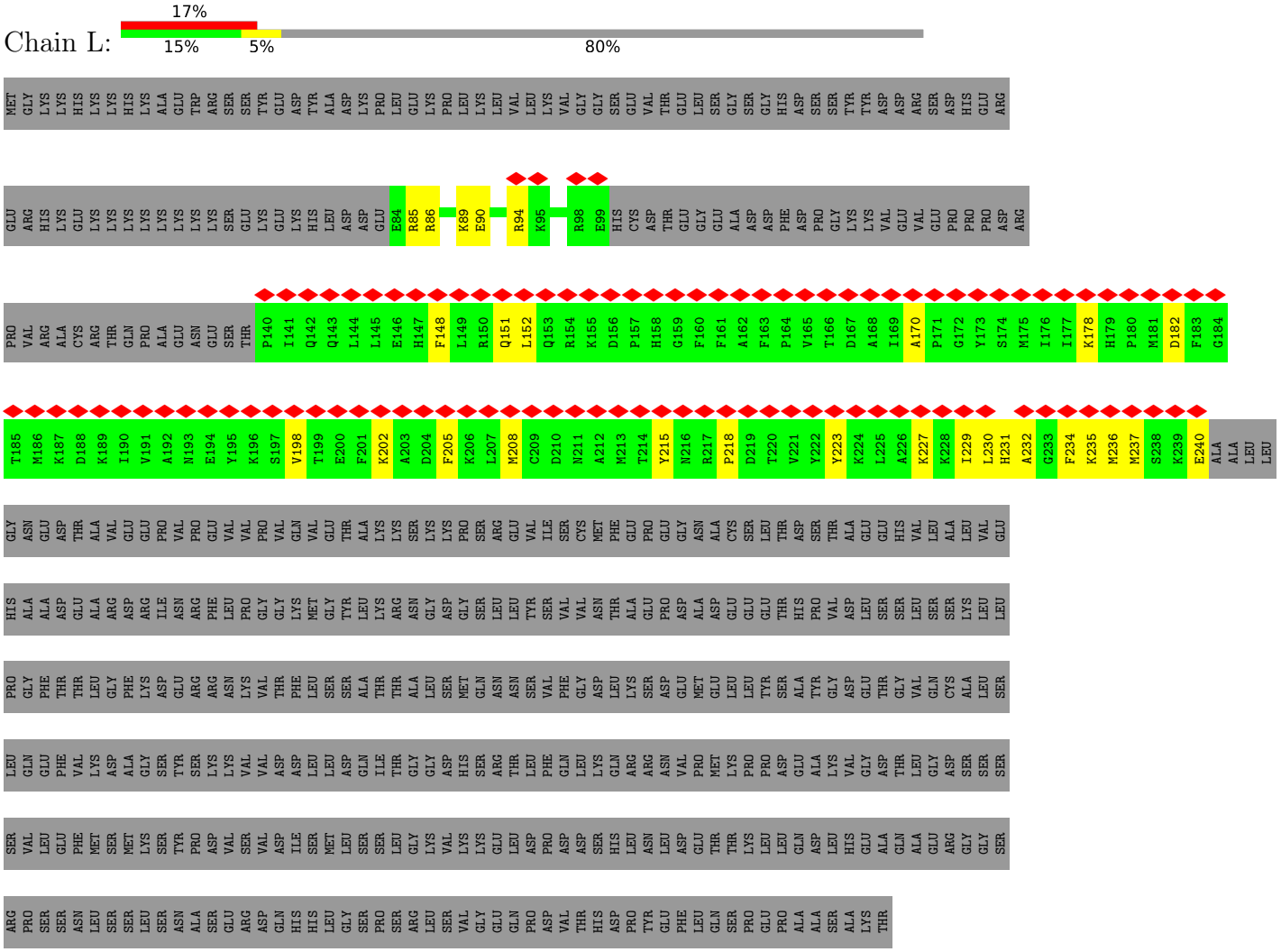
• Molecule 7: DNA (131-MER)

Chain J:

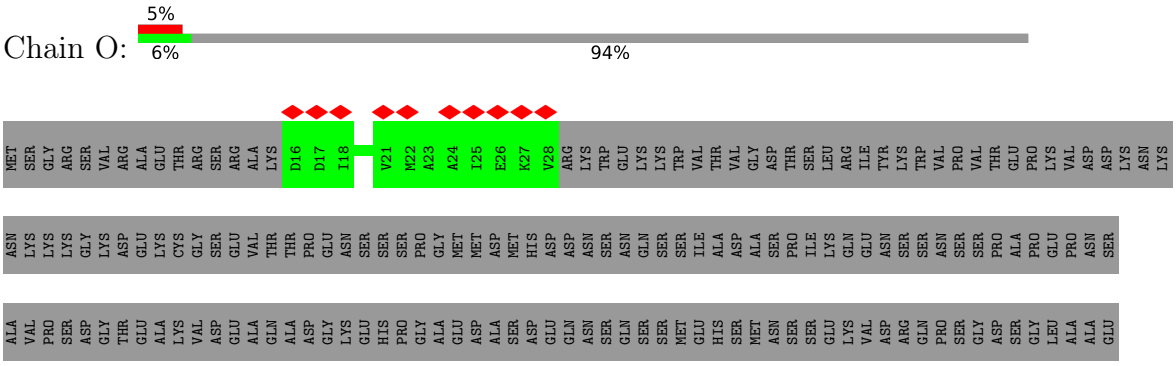




• Molecule 8: Bromodomain-containing protein 9

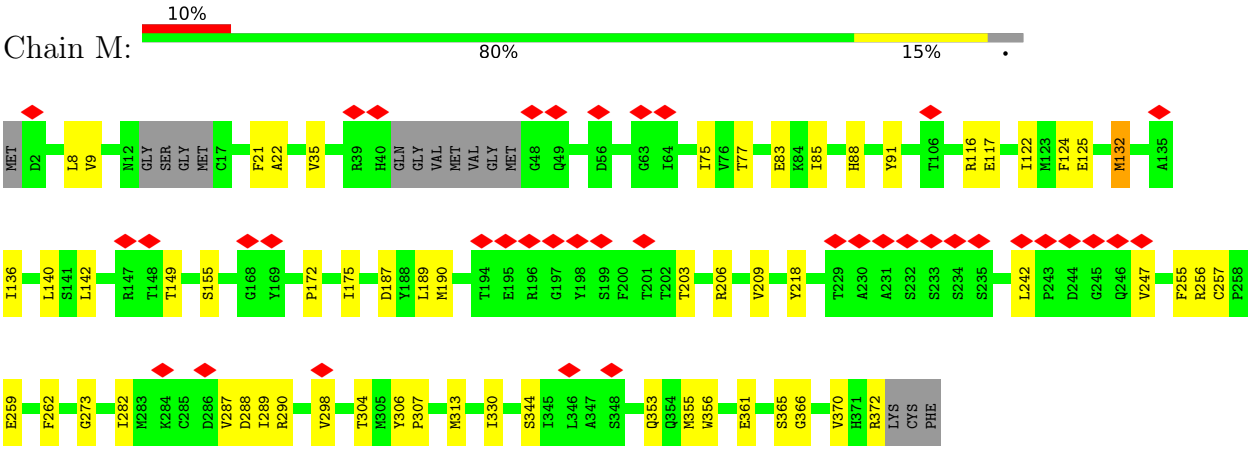


• Molecule 9: B-cell CLL/lymphoma 7 protein family member A

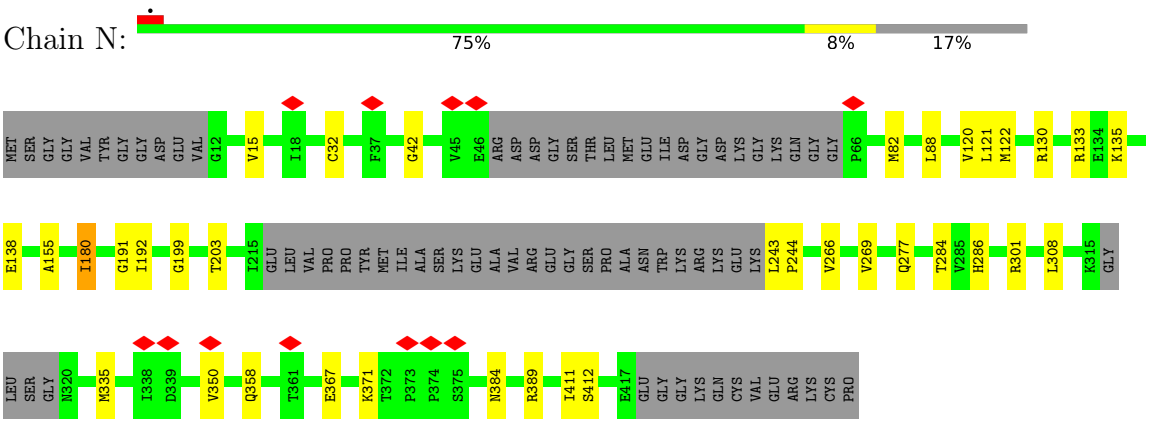




• Molecule 10: Actin, cytoplasmic 1, N-terminally processed



• Molecule 11: Actin-like protein 6A



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	35.532	Depositor
Minimum map value	-6.182	Depositor
Average map value	0.099	Depositor
Map value standard deviation	0.631	Depositor
Recommended contour level	2	Depositor
Map size (Å)	320.768, 320.768, 320.768	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.253, 1.253, 1.253	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	K	0.13	0/5539	0.34	0/7447
2	A	0.16	0/813	0.32	0/1090
2	E	0.40	1/811 (0.1%)	0.54	2/1086 (0.2%)
3	B	0.15	0/669	0.35	0/894
3	F	0.17	0/626	0.31	0/837
4	C	0.14	0/805	0.27	0/1088
4	G	0.13	0/819	0.26	0/1106
5	D	0.14	0/756	0.28	0/1015
5	H	0.13	0/737	0.27	0/993
6	I	0.80	0/2990	0.94	0/4608
7	J	0.77	0/3034	0.89	0/4685
8	L	0.34	0/1018	0.53	0/1354
9	O	0.06	0/64	0.24	0/88
10	M	0.12	0/2881	0.34	0/3904
11	N	0.12	0/2849	0.31	0/3866
All	All	0.42	1/24411 (0.0%)	0.56	2/34061 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	81	ASP	N-CA	5.30	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	77	ASP	CA-C-N	-5.27	113.95	122.23
2	E	77	ASP	C-N-CA	-5.27	113.95	122.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	78	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	5439	0	5519	38	0
2	A	801	0	839	1	0
2	E	800	0	835	41	0
3	B	662	0	709	2	0
3	F	619	0	659	7	0
4	C	795	0	846	4	0
4	G	809	0	864	3	0
5	D	745	0	773	5	0
5	H	726	0	747	7	0
6	I	2669	0	1471	37	0
7	J	2702	0	1471	32	0
8	L	988	0	1006	47	0
9	O	65	0	31	0	0
10	M	2821	0	2780	31	0
11	N	2787	0	2725	20	0
12	K	27	0	12	0	0
13	K	1	0	0	0	0
14	K	4	0	0	0	0
All	All	23460	0	21287	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:LYS:O	8:L:235:LYS:HB2	1.80	0.81
2:E:81:ASP:C	8:L:231:HIS:HD1	1.89	0.80
2:E:80:THR:C	8:L:231:HIS:HD1	1.90	0.80
2:E:80:THR:C	8:L:231:HIS:ND1	2.31	0.78
7:J:-20:DC:H2'	7:J:-19:DG:C8	2.19	0.77
2:E:79:LYS:HG2	2:E:82:LEU:HG	1.67	0.75
11:N:277:GLN:HA	11:N:301:ARG:HH12	1.50	0.74
2:E:82:LEU:HG	8:L:231:HIS:CE1	2.23	0.73
2:E:79:LYS:O	8:L:232:ALA:HA	1.90	0.71
10:M:189:LEU:HD13	10:M:209:VAL:HG22	1.72	0.69
6:I:22:DC:H2'	6:I:23:DA:C8	2.30	0.67
1:K:806:PHE:HB2	1:K:855:VAL:HG12	1.76	0.67
8:L:218:PRO:HA	8:L:223:TYR:CG	2.33	0.64
1:K:1228:VAL:HG13	1:K:1229:ILE:HG13	1.80	0.64
10:M:122:ILE:HA	10:M:125:GLU:HG2	1.80	0.64
2:E:80:THR:HG22	2:E:80:THR:O	1.97	0.63
10:M:83:GLU:HG2	10:M:122:ILE:HD11	1.81	0.63
2:E:79:LYS:C	8:L:235:LYS:HB2	2.23	0.63
10:M:117:GLU:HG3	10:M:366:GLY:HA3	1.81	0.63
7:J:21:DG:H2'	7:J:22:DT:H71	1.81	0.62
6:I:30:DT:H2'	6:I:31:DT:H71	1.81	0.62
7:J:49:DC:H2"	7:J:50:DG:C8	2.34	0.62
2:E:77:ASP:C	8:L:234:PHE:HB3	2.26	0.61
7:J:7:DC:H2"	7:J:8:DG:C8	2.35	0.61
10:M:203:THR:HA	10:M:206:ARG:HB2	1.82	0.60
7:J:37:DC:H2"	7:J:38:DG:C8	2.37	0.60
2:E:79:LYS:CE	2:E:80:THR:H	2.15	0.60
2:E:81:ASP:CA	8:L:231:HIS:HD1	2.06	0.60
7:J:-24:DT:H2'	7:J:-23:DT:H71	1.84	0.59
2:E:81:ASP:CA	8:L:231:HIS:ND1	2.60	0.58
7:J:-54:DC:H2"	7:J:-53:DA:C8	2.38	0.58
6:I:38:DT:H2"	6:I:39:DA:C8	2.39	0.58
4:C:42:ARG:HG3	5:D:85:THR:HG23	1.85	0.58
6:I:-26:DT:H2"	6:I:-25:DA:C8	2.38	0.58
8:L:205:PHE:O	8:L:208[B]:MET:HG2	2.04	0.57
6:I:-7:DG:H2"	6:I:-6:DT:H71	1.85	0.57
2:E:81:ASP:C	8:L:231:HIS:ND1	2.58	0.57
10:M:262:PHE:HB2	10:M:273:GLY:HA3	1.87	0.57
2:E:121:PRO:HB3	3:F:53:GLU:HG3	1.86	0.57
6:I:-57:DC:H2"	6:I:-56:DC:C5	2.40	0.57
2:E:79:LYS:O	8:L:231:HIS:C	2.48	0.57
5:H:106:HIS:CD2	8:L:85:ARG:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:75:ALA:HB1	2:E:82:LEU:HD12	1.86	0.56
2:E:79:LYS:HG3	2:E:80:THR:N	2.19	0.56
3:F:54:THR:HA	3:F:57:VAL:HG22	1.87	0.56
4:C:30:VAL:HG13	5:D:67:PHE:HE2	1.70	0.56
4:G:102:ILE:HG23	5:H:58:ILE:HD13	1.87	0.56
7:J:-65:DT:H2"	7:J:-64:DA:C8	2.40	0.56
11:N:191:GLY:HA2	11:N:335:MET:HE3	1.88	0.55
2:E:79:LYS:HE2	2:E:80:THR:H	1.70	0.55
8:L:151:GLN:HB3	8:L:236[B]:MET:SD	2.46	0.55
2:E:81:ASP:OD1	8:L:227:LYS:HE2	2.07	0.55
6:I:-27:DC:H2"	6:I:-26:DT:H71	1.87	0.55
11:N:266:VAL:HG12	11:N:358:GLN:HB2	1.89	0.55
2:E:77:ASP:O	8:L:234:PHE:HB3	2.06	0.54
10:M:22:ALA:HB1	10:M:344:SER:HA	1.90	0.54
6:I:-25:DA:H2"	6:I:-24:DG:C8	2.43	0.54
6:I:-6:DT:H2"	6:I:-5:DA:C8	2.43	0.53
6:I:53:DT:H2"	6:I:54:DG:C8	2.43	0.53
5:D:102:GLU:HA	5:D:105:LYS:HG2	1.90	0.53
6:I:49:DC:H2"	6:I:50:DA:C8	2.43	0.53
6:I:-4:DC:H2"	6:I:-3:DG:C8	2.44	0.53
1:K:967:ARG:HA	1:K:971:VAL:HG22	1.90	0.53
1:K:896:VAL:O	1:K:900:HIS:HB3	2.09	0.53
1:K:500:LEU:HD11	10:M:142:LEU:HD23	1.91	0.53
8:L:205:PHE:HZ	8:L:229:ILE:O	1.91	0.53
5:H:105:LYS:HD3	8:L:86:ARG:NH2	2.24	0.53
7:J:-21:DG:OP1	8:L:218:PRO:HG2	2.10	0.52
10:M:353:GLN:HA	10:M:356:TRP:CD1	2.45	0.52
2:E:82:LEU:HG	8:L:231:HIS:HE1	1.74	0.52
1:K:996:ILE:HG12	1:K:1305:MET:HE1	1.91	0.52
7:J:15:DT:H2"	7:J:16:DA:C8	2.45	0.52
8:L:202:LYS:HB3	8:L:234:PHE:CE2	2.45	0.51
10:M:75:ILE:HG22	10:M:77:THR:H	1.74	0.51
2:E:77:ASP:HA	8:L:234:PHE:CG	2.46	0.51
6:I:-31:DA:H2"	6:I:-30:DG:H8	1.76	0.51
1:K:1003:LEU:HA	1:K:1006:VAL:HG22	1.93	0.51
6:I:22:DC:H2"	6:I:23:DA:H5'	1.92	0.51
10:M:136:ILE:O	10:M:140:LEU:HD23	2.11	0.51
11:N:155:ALA:HB2	11:N:180:ILE:HD12	1.93	0.51
1:K:1108:LEU:HD21	1:K:1174:PHE:CE1	2.46	0.51
6:I:-38:DC:H2"	6:I:-37:DG:C8	2.45	0.51
7:J:49:DC:H2"	7:J:50:DG:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:834:TYR:HB2	1:K:856:LEU:HD11	1.92	0.50
1:K:994:TYR:HB3	1:K:1305:MET:HE3	1.94	0.50
10:M:298:VAL:HG12	10:M:330:ILE:HB	1.94	0.50
1:K:1101:LEU:HD21	1:K:1112:MET:HE2	1.94	0.50
1:K:878:MET:HB3	1:K:906:ARG:HG2	1.94	0.50
2:E:79:LYS:O	8:L:231:HIS:O	2.30	0.49
2:E:63:ARG:NH1	7:J:-14:DA:H4'	2.27	0.49
2:E:79:LYS:C	8:L:231:HIS:CD2	2.91	0.49
10:M:256:ARG:O	10:M:259:GLU:HB2	2.11	0.49
11:N:180:ILE:HG22	11:N:192:ILE:HG12	1.94	0.49
1:K:967:ARG:HE	1:K:1228:VAL:HG23	1.77	0.49
2:E:79:LYS:CG	2:E:80:THR:N	2.75	0.49
1:K:888:ASN:HB3	1:K:891:CYS:SG	2.53	0.49
3:F:31:LYS:HG3	3:F:51:TYR:CZ	2.48	0.49
1:K:789:THR:O	1:K:793:ILE:HG12	2.13	0.48
10:M:9:VAL:HG23	10:M:22:ALA:HB2	1.94	0.48
6:I:64:DT:H2"	6:I:65:DA:C8	2.49	0.48
10:M:361:GLU:O	10:M:365:SER:HB3	2.14	0.48
7:J:-2:DC:H2"	7:J:-1:DA:C8	2.49	0.47
8:L:182:ASP:HA	8:L:208[B]:MET:HE3	1.96	0.47
6:I:62:DT:H2"	6:I:63:DA:C8	2.49	0.47
7:J:-17:DT:H4'	7:J:-16:DT:OP1	2.12	0.47
2:E:81:ASP:CG	2:E:81:ASP:O	2.57	0.47
7:J:-25:DC:H2"	7:J:-24:DT:H72	1.95	0.47
10:M:8:LEU:HD13	10:M:21:PHE:HA	1.97	0.47
10:M:124:PHE:HB2	10:M:132:MET:SD	2.54	0.47
1:K:969:HIS:CD2	1:K:1243:ARG:HH21	2.33	0.47
10:M:304:THR:HA	10:M:306:TYR:CE2	2.50	0.47
2:E:80:THR:N	8:L:235:LYS:HE2	2.29	0.47
8:L:230:LEU:O	8:L:231:HIS:C	2.56	0.47
6:I:-23:DC:H2"	6:I:-22:DA:H8	1.80	0.46
6:I:35:DC:H2"	6:I:36:DC:C5	2.50	0.46
2:E:79:LYS:CA	8:L:231:HIS:CD2	2.95	0.46
2:E:79:LYS:C	8:L:231:HIS:CG	2.94	0.46
1:K:557:THR:HA	1:K:560:TYR:HD2	1.80	0.46
2:E:79:LYS:CA	8:L:235:LYS:HB2	2.46	0.46
1:K:965:ILE:HA	1:K:968:LEU:HB2	1.98	0.46
1:K:1039:ILE:HG13	1:K:1210:VAL:HG21	1.97	0.46
6:I:-47:DT:H2"	6:I:-46:DC:C5	2.51	0.46
7:J:-18:DG:C8	7:J:-18:DG:H5'	2.50	0.46
10:M:35:VAL:HG22	10:M:85:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:88:LEU:HD23	11:N:88:LEU:H	1.81	0.46
1:K:884:HIS:O	1:K:887:LYS:HG3	2.16	0.45
1:K:1048:HIS:CD2	1:K:1050:TYR:HB2	2.51	0.45
2:E:82:LEU:HD11	3:F:70:VAL:HG22	1.97	0.45
7:J:-22:DG:H2"	7:J:-21:DG:OP2	2.16	0.45
10:M:287:VAL:HG22	10:M:288:ASP:H	1.80	0.45
8:L:236[B]:MET:HE2	8:L:236[B]:MET:HB3	1.70	0.45
10:M:282:ILE:HG22	10:M:290:ARG:HG3	1.99	0.45
11:N:243:LEU:HB2	11:N:244:PRO:HD3	1.98	0.45
6:I:44:DC:H2"	6:I:45:DC:C6	2.52	0.45
6:I:-43:DT:H2'	6:I:-42:DT:H71	1.98	0.45
6:I:22:DC:H2'	6:I:23:DA:H8	1.77	0.45
11:N:15:VAL:HG12	11:N:121:LEU:HB3	1.98	0.45
8:L:205:PHE:CZ	8:L:229:ILE:O	2.69	0.45
11:N:199:GLY:O	11:N:203:THR:HG23	2.17	0.45
4:C:102:ILE:HG23	5:D:58:ILE:HD13	1.99	0.45
11:N:42:GLY:HA3	11:N:82:MET:HB3	1.99	0.45
6:I:4:DC:H2"	6:I:5:DC:C6	2.51	0.45
7:J:-9:DC:H2"	7:J:-8:DG:C8	2.51	0.45
6:I:-31:DA:H2"	6:I:-30:DG:C8	2.51	0.45
3:F:89:ALA:O	3:F:93:GLN:HG2	2.16	0.45
1:K:917:LYS:O	1:K:920:GLU:HG2	2.17	0.44
7:J:-63:DT:H2"	7:J:-62:DA:H8	1.82	0.44
10:M:172:PRO:HD2	11:N:32:CYS:SG	2.57	0.44
4:G:84:GLN:HE21	4:G:105:GLY:HA3	1.82	0.44
1:K:1227:LYS:HG2	1:K:1250:ILE:HD13	2.00	0.44
4:C:109:PRO:HA	2:E:55:GLN:HG2	1.98	0.44
10:M:255:PHE:O	10:M:259:GLU:HG3	2.17	0.44
6:I:0:DC:H2'	6:I:1:DT:H71	2.00	0.44
7:J:-17:DT:H2"	7:J:-16:DT:O5'	2.18	0.44
1:K:1295:GLU:O	1:K:1296:VAL:HG13	2.18	0.44
7:J:-63:DT:H2"	7:J:-62:DA:C8	2.52	0.44
8:L:178:LYS:HA	8:L:178:LYS:HD3	1.84	0.44
10:M:187:ASP:O	10:M:190:MET:HG3	2.18	0.44
11:N:120:VAL:HG12	11:N:122:MET:HE3	2.00	0.44
1:K:496:LYS:HE3	10:M:355:MET:HG2	1.98	0.44
11:N:367:GLU:O	11:N:371:LYS:HG2	2.18	0.44
1:K:492:SER:O	1:K:496:LYS:HG2	2.18	0.43
2:E:79:LYS:CD	2:E:80:THR:H	2.31	0.43
2:E:76:GLN:HG3	8:L:230:LEU:HG	2.00	0.43
8:L:202:LYS:HG2	8:L:237:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-14:DA:H2"	6:I:-13:DA:C8	2.53	0.43
6:I:-44:DA:C2'	6:I:-43:DT:H71	2.48	0.43
7:J:-22:DG:C2	7:J:-21:DG:C5	3.06	0.43
1:K:861:GLU:HG2	6:I:-18:DC:H4'	2.01	0.43
6:I:-23:DC:H2"	6:I:-22:DA:C8	2.54	0.43
1:K:764:TRP:CH2	1:K:768:LEU:HD11	2.54	0.43
6:I:69:DC:H2"	6:I:70:DG:C8	2.54	0.43
7:J:27:DG:H2"	7:J:28:DA:C8	2.53	0.43
8:L:198:VAL:HG12	8:L:202:LYS:HE3	2.01	0.43
11:N:284:THR:HG23	11:N:286:HIS:H	1.84	0.43
11:N:308:LEU:HD23	11:N:308:LEU:H	1.84	0.43
5:H:106:HIS:ND1	8:L:89:LYS:HD3	2.34	0.43
6:I:-14:DA:H2"	6:I:-13:DA:H8	1.83	0.43
8:L:236[A]:MET:HE3	8:L:236[A]:MET:HB3	1.84	0.42
5:H:105:LYS:NZ	8:L:86:ARG:HH12	2.17	0.42
6:I:36:DC:H2"	6:I:37:DC:C5	2.54	0.42
11:N:411:ILE:HG22	11:N:412:SER:H	1.84	0.42
7:J:-2:DC:H2"	7:J:-1:DA:H8	1.84	0.42
10:M:218:TYR:HA	10:M:307:PRO:HD2	2.01	0.42
11:N:350:VAL:O	11:N:389:ARG:HD3	2.19	0.42
2:E:107:THR:HG23	2:E:123:ASP:HB2	2.01	0.42
1:K:776:ILE:HD13	1:K:908:LEU:HB2	2.02	0.42
3:F:35:ARG:O	3:F:39:ARG:HG2	2.20	0.42
6:I:49:DC:H2"	6:I:50:DA:H8	1.84	0.42
7:J:38:DG:H2"	7:J:39:DA:C8	2.55	0.42
10:M:116:ARG:HG2	10:M:370:VAL:HG13	2.02	0.42
3:B:31:LYS:HG3	3:B:51:TYR:CE1	2.54	0.42
2:E:79:LYS:C	8:L:235:LYS:HE2	2.45	0.42
5:H:105:LYS:HD3	8:L:86:ARG:HH22	1.85	0.42
3:B:56:GLY:O	3:B:59:LYS:HG2	2.20	0.42
7:J:-69:DG:H2"	7:J:-68:DA:C8	2.55	0.42
2:E:82:LEU:N	8:L:231:HIS:ND1	2.67	0.41
7:J:34:DC:H6	7:J:34:DC:H2'	1.72	0.41
8:L:170:ALA:HB1	8:L:215:TYR:CZ	2.55	0.41
1:K:749:MET:HE3	1:K:790:ILE:HG13	2.01	0.41
4:G:40:ALA:HB2	5:H:86:ILE:HG13	2.02	0.41
2:E:78:PHE:HB3	3:F:70:VAL:HG11	2.03	0.41
6:I:-2:DC:H2"	6:I:-1:DG:C8	2.55	0.41
7:J:-5:DG:H2"	7:J:-4:DG:C8	2.55	0.41
8:L:90:GLU:O	8:L:94:ARG:HG2	2.21	0.41
5:D:41:VAL:O	5:D:45:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-47:DC:H2"	7:J:-46:DT:C5	2.56	0.41
11:N:130:ARG:HA	11:N:133:ARG:HG2	2.03	0.41
1:K:1183:ASP:O	1:K:1187:GLN:HG3	2.20	0.41
6:I:8:DC:H2"	6:I:9:DG:C8	2.56	0.41
6:I:55:DT:H2"	6:I:56:DC:C5	2.54	0.41
1:K:749:MET:HE2	1:K:825:TRP:CE3	2.56	0.41
2:E:65:LEU:HB3	2:E:66:PRO:HD3	2.02	0.41
7:J:-21:DG:OP2	7:J:-21:DG:H8	2.04	0.41
10:M:313:MET:HE2	10:M:313:MET:HB2	1.95	0.41
1:K:915:GLN:HB3	1:K:1179:ASN:HD21	1.86	0.41
7:J:16:DA:H2"	7:J:17:DA:C8	2.56	0.40
8:L:148:PHE:O	8:L:152:LEU:HG	2.22	0.40
11:N:135:LYS:O	11:N:138:GLU:HG2	2.22	0.40
1:K:962:ILE:HA	1:K:965:ILE:HG12	2.03	0.40
10:M:287:VAL:HG13	10:M:289:ILE:H	1.85	0.40
11:N:384:ASN:HA	11:N:389:ARG:HD2	2.02	0.40
1:K:489:TYR:HB2	10:M:372:ARG:HE	1.86	0.40
1:K:502:LYS:O	1:K:506:THR:HG23	2.21	0.40
1:K:918:LEU:N	1:K:919:PRO:HD2	2.36	0.40
7:J:17:DA:H2"	7:J:18:DG:H8	1.87	0.40
10:M:88:HIS:O	10:M:91:TYR:HB2	2.21	0.40
1:K:1008:TYR:CE2	1:K:1042:LEU:HD22	2.57	0.40
2:A:47:ALA:O	2:A:51:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	641/1647 (39%)	616 (96%)	25 (4%)	0	100	100
2	A	95/136 (70%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	95/136 (70%)	93 (98%)	1 (1%)	1 (1%)	11	22
3	B	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
3	F	76/103 (74%)	76 (100%)	0	0	100	100
4	C	101/130 (78%)	101 (100%)	0	0	100	100
4	G	103/130 (79%)	103 (100%)	0	0	100	100
5	D	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
5	H	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
8	L	116/597 (19%)	114 (98%)	2 (2%)	0	100	100
9	O	11/210 (5%)	10 (91%)	1 (9%)	0	100	100
10	M	354/375 (94%)	330 (93%)	24 (7%)	0	100	100
11	N	348/429 (81%)	324 (93%)	24 (7%)	0	100	100
All	All	2205/4248 (52%)	2120 (96%)	84 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	81	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	592/1422 (42%)	588 (99%)	4 (1%)	76	86
2	A	85/111 (77%)	85 (100%)	0	100	100
2	E	84/111 (76%)	78 (93%)	6 (7%)	13	25
3	B	68/79 (86%)	68 (100%)	0	100	100
3	F	63/79 (80%)	63 (100%)	0	100	100
4	C	82/101 (81%)	82 (100%)	0	100	100
4	G	83/101 (82%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	D	81/106 (76%)	81 (100%)	0	100 100
5	H	79/106 (74%)	79 (100%)	0	100 100
8	L	106/527 (20%)	105 (99%)	1 (1%)	70 82
10	M	307/318 (96%)	300 (98%)	7 (2%)	44 66
11	N	308/364 (85%)	306 (99%)	2 (1%)	78 88
All	All	1938/3425 (57%)	1918 (99%)	20 (1%)	65 81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	773	LEU
1	K	900	HIS
1	K	1154	LEU
1	K	1296	VAL
2	E	55	GLN
2	E	79	LYS
2	E	81	ASP
2	E	82	LEU
2	E	112	ILE
2	E	125	GLN
8	L	240	GLU
10	M	132	MET
10	M	149	THR
10	M	155	SER
10	M	175	ILE
10	M	242	LEU
10	M	247	VAL
10	M	257	CYS
11	N	180	ILE
11	N	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	470	GLN
1	K	481	GLN
1	K	519	ASN
1	K	751	ASN
1	K	847	GLN

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Mol	Chain	Res	Type
1	K	969	HIS
1	K	1187	GLN
5	D	46	HIS
5	D	92	GLN
2	E	85	GLN
3	F	27	GLN
4	G	24	GLN
4	G	68	ASN
4	G	73	ASN
5	H	92	GLN
10	M	92	ASN
10	M	115	ASN
11	N	105	HIS
11	N	143	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	ADP	K	1701	13	27,29,29	1.34	4 (14%)	42,45,45	1.95	10 (23%)
14	BEF	K	1703	-	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ADP	K	1701	13	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	1701	ADP	C5-C4	4.40	1.47	1.39
12	K	1701	ADP	C5-C6	2.64	1.48	1.41
12	K	1701	ADP	C8-N7	2.34	1.36	1.31
12	K	1701	ADP	C5-N7	-2.16	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	1701	ADP	C5-C4-N3	-6.03	118.88	126.75
12	K	1701	ADP	N3-C4-N9	4.75	134.91	127.08
12	K	1701	ADP	C2-N3-C4	3.84	120.82	111.75
12	K	1701	ADP	PA-O3A-PB	-3.33	121.41	132.83
12	K	1701	ADP	C4-C5-N7	-3.25	106.66	110.62
12	K	1701	ADP	N3-C2-N1	-3.18	123.63	128.60
12	K	1701	ADP	C5-N7-C8	2.75	107.42	103.51
12	K	1701	ADP	C4-N9-C8	2.74	108.70	105.73
12	K	1701	ADP	C6-C5-N7	2.27	136.25	132.02
12	K	1701	ADP	N9-C8-N7	-2.13	111.01	113.91

There are no chirality outliers.

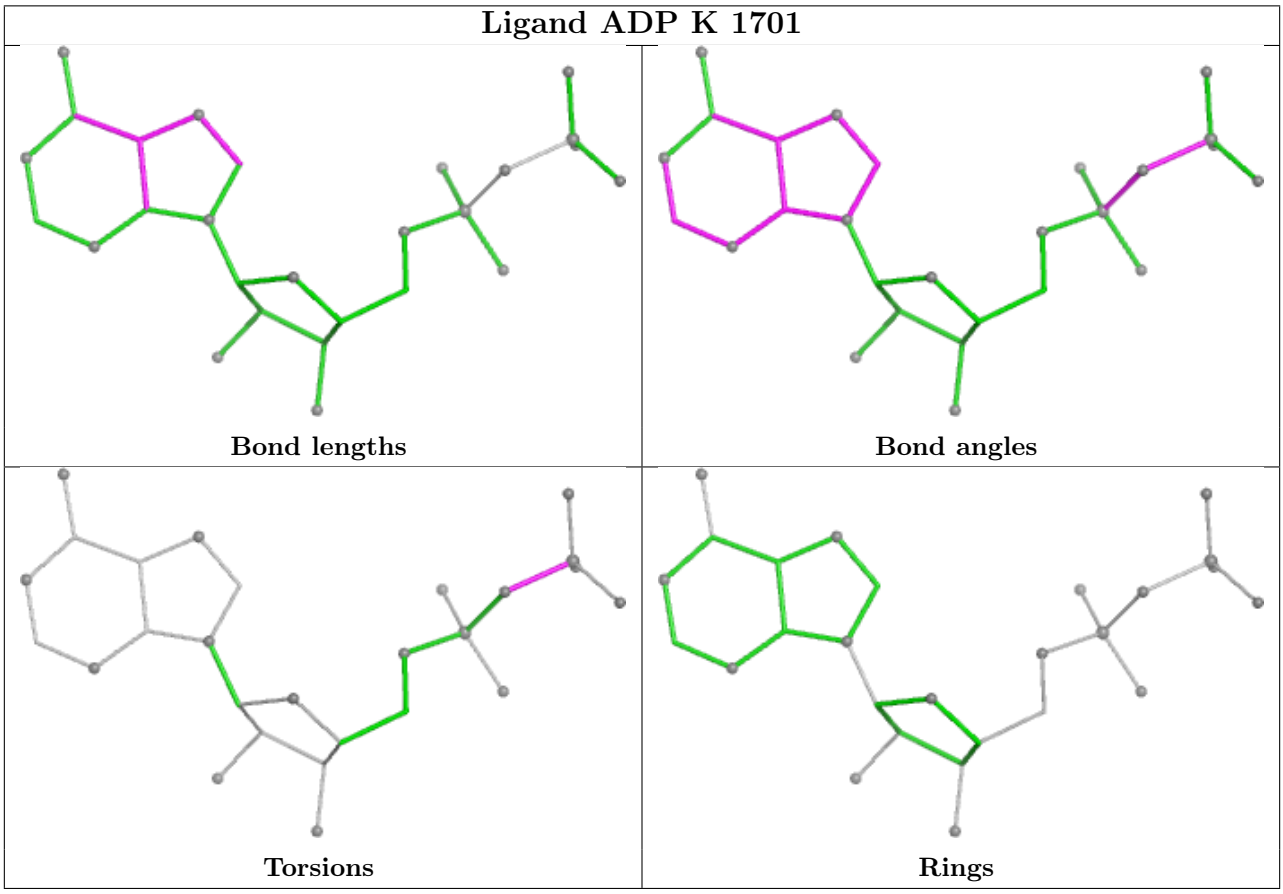
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	K	1701	ADP	PA-O3A-PB-O2B
12	K	1701	ADP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

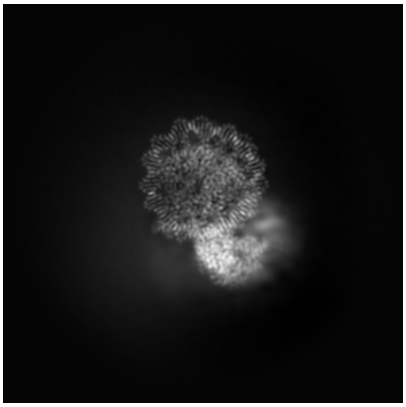
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55887. These allow visual inspection of the internal detail of the map and identification of artifacts.

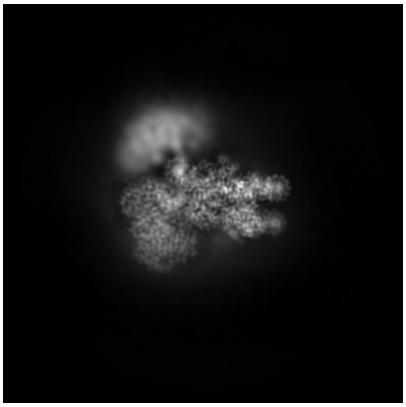
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

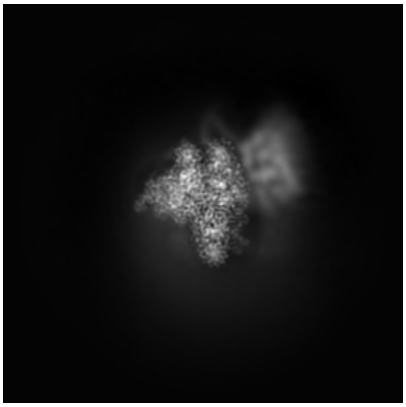
6.1.1 Primary map



X



Y



Z

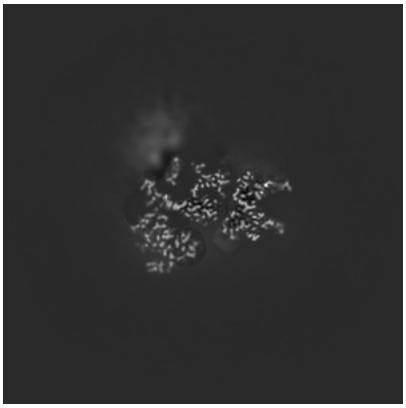
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 128



Y Index: 128

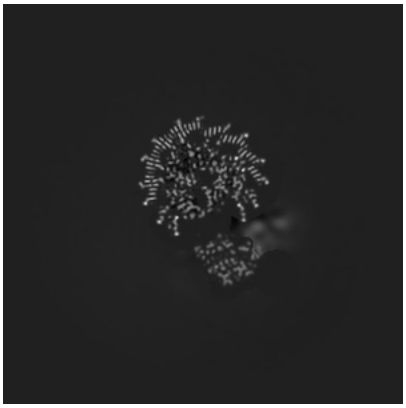


Z Index: 128

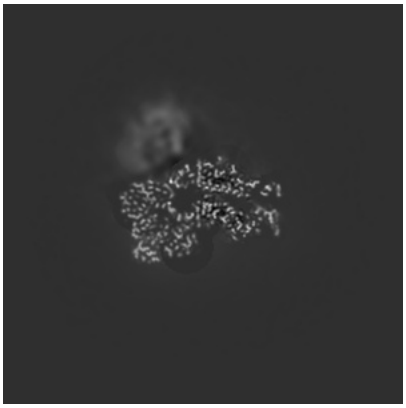
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 136



Y Index: 139

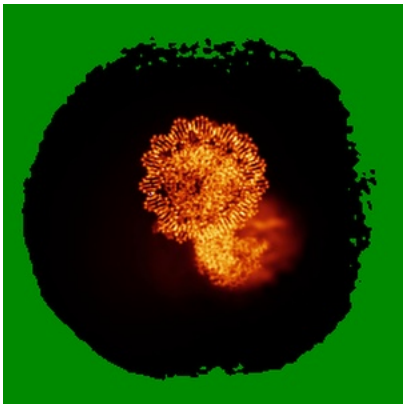


Z Index: 113

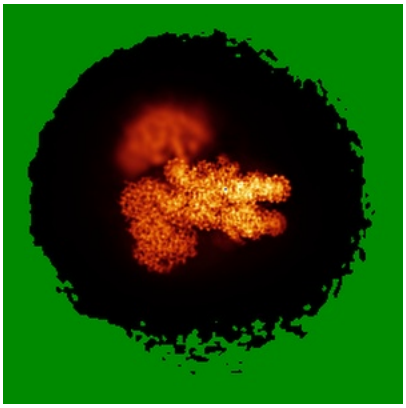
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

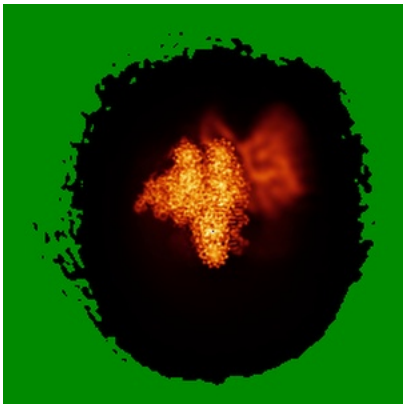
6.4.1 Primary map



X



Y

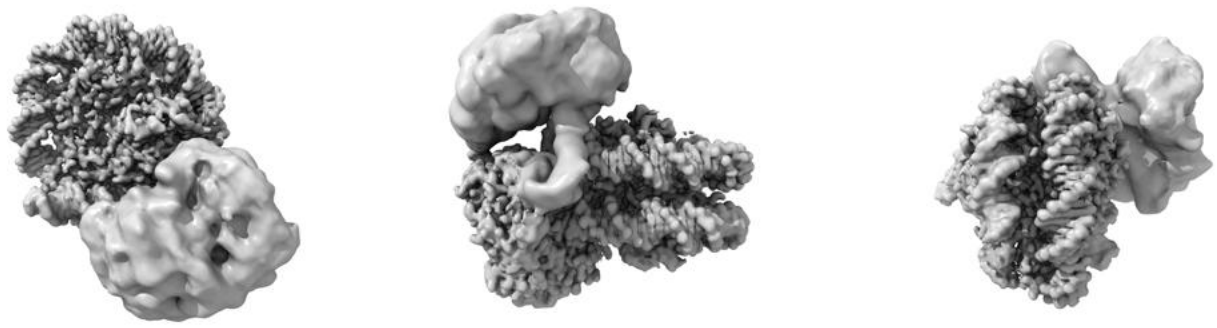


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

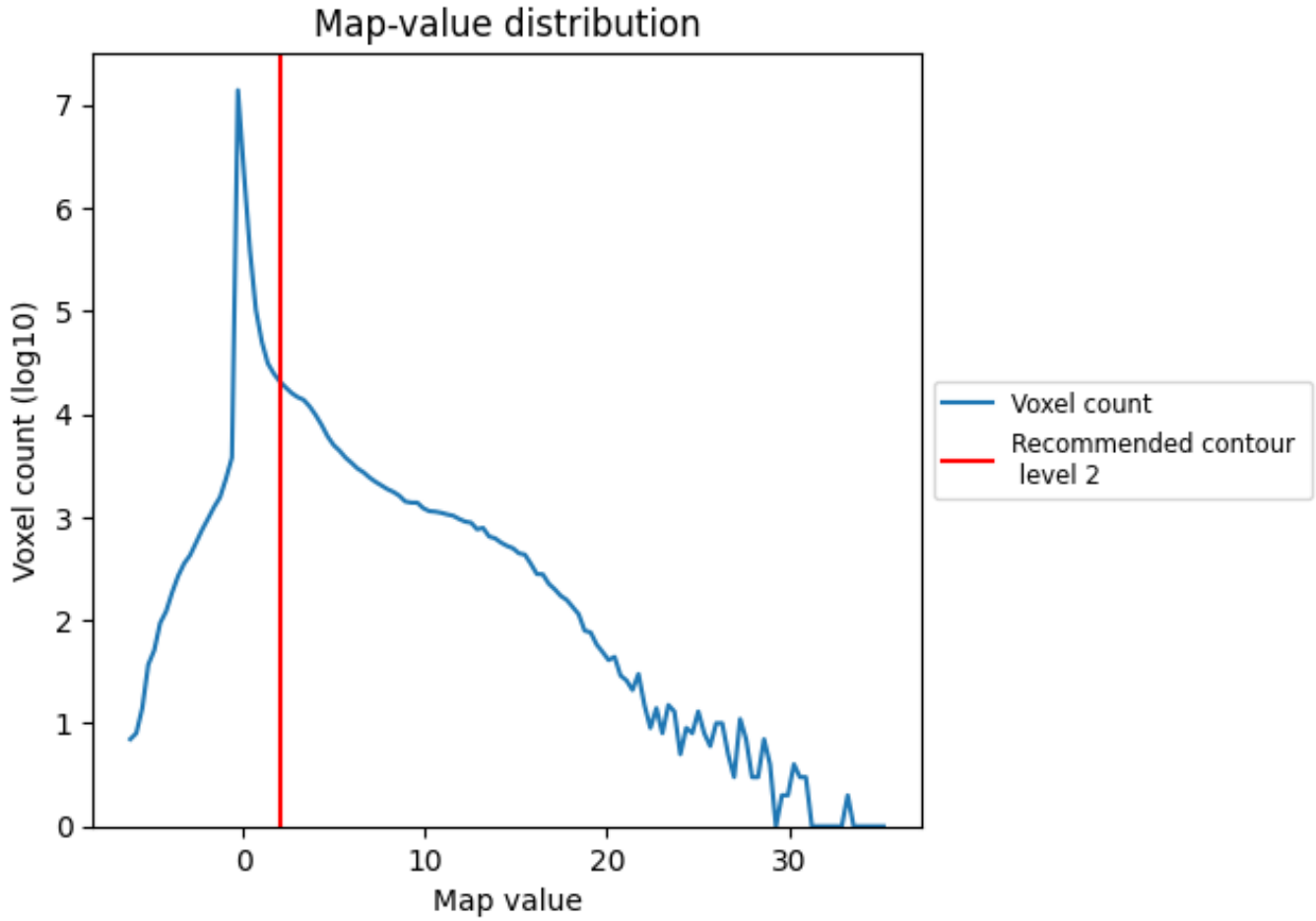
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

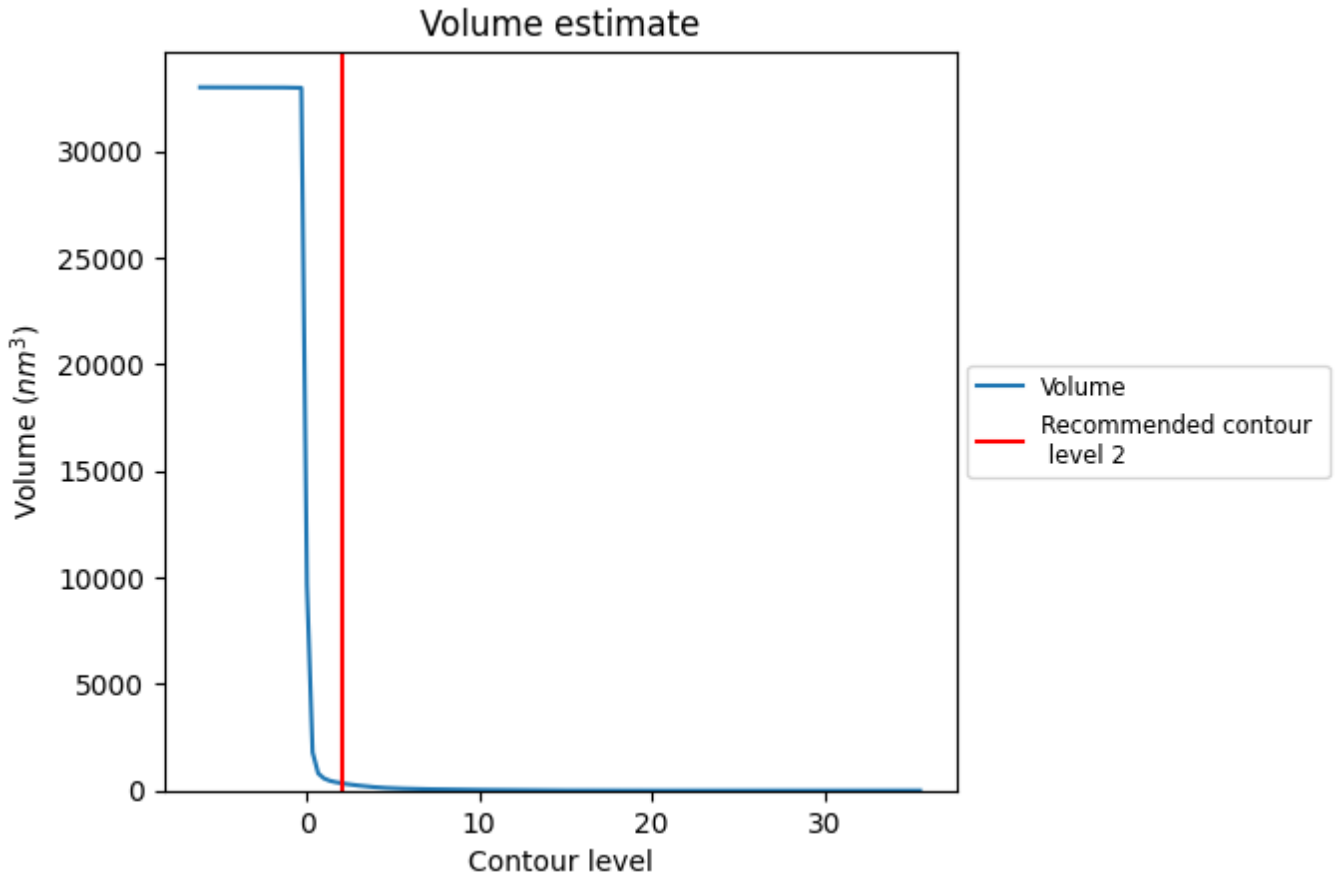
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

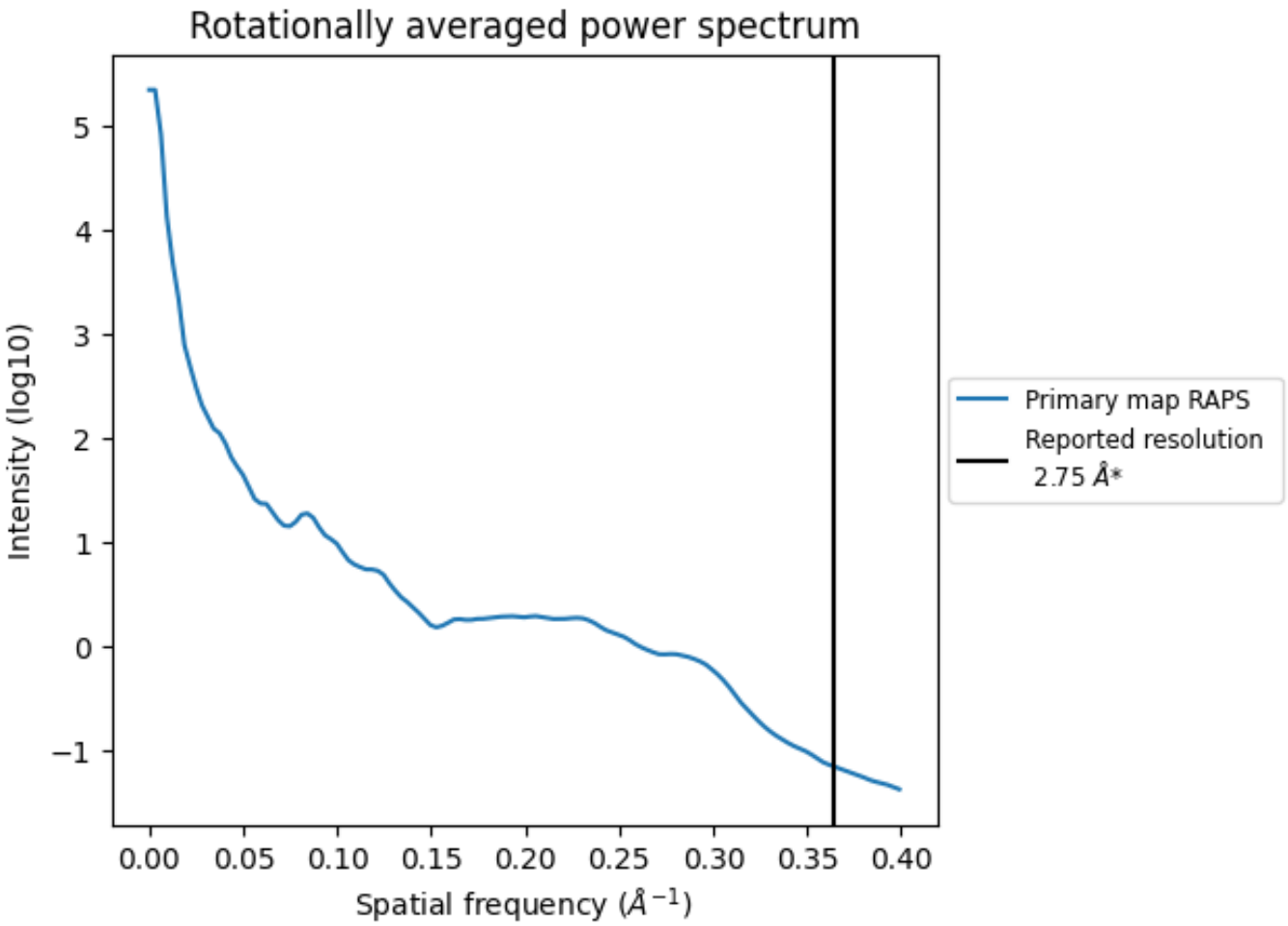
7.2 Volume estimate



The volume at the recommended contour level is 346 nm^3; this corresponds to an approximate mass of 313 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

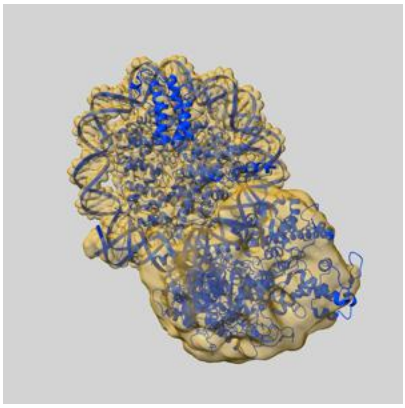
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

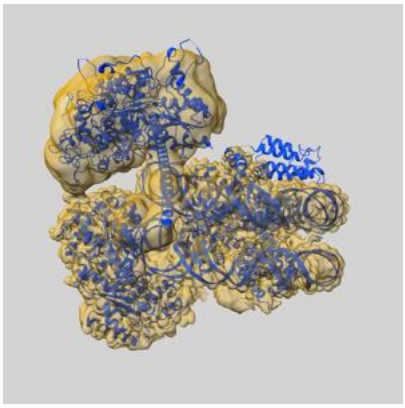
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55887 and PDB model 9TG1. Per-residue inclusion information can be found in section 3 on page 8.

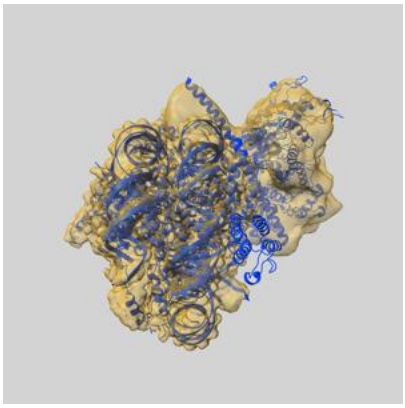
9.1 Map-model overlay



X



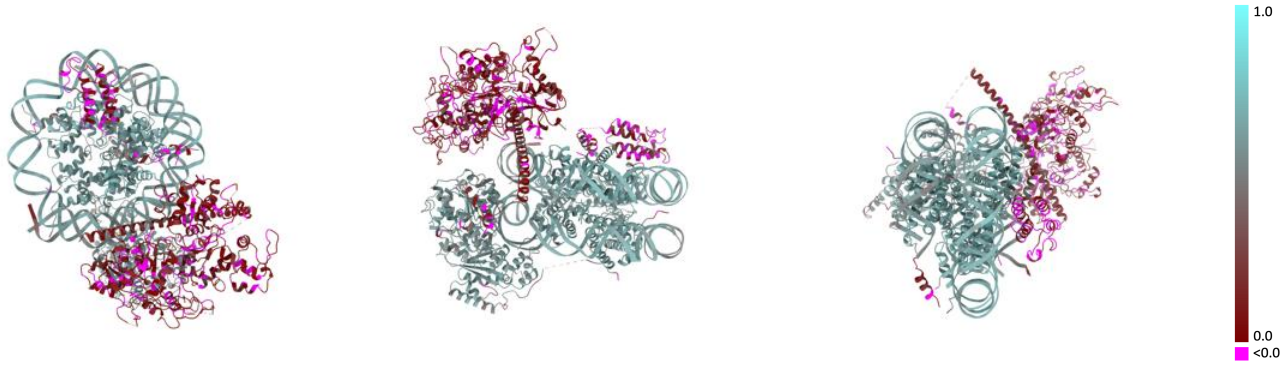
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

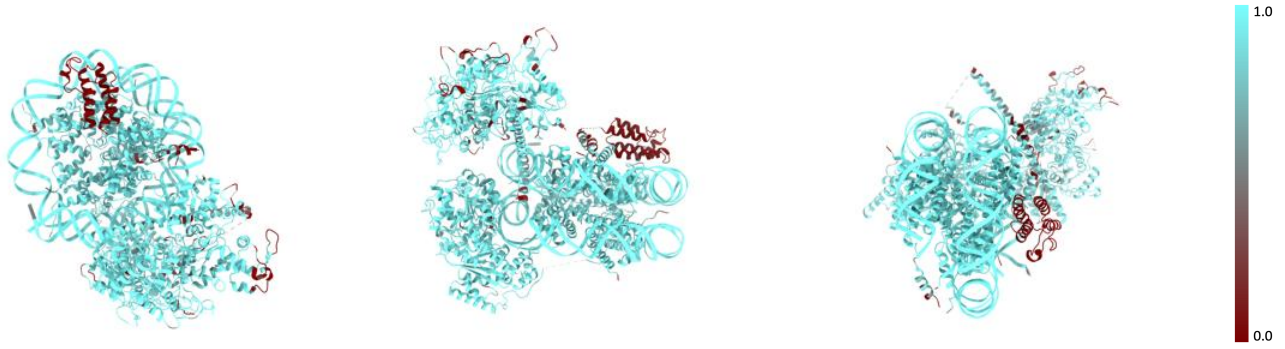
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

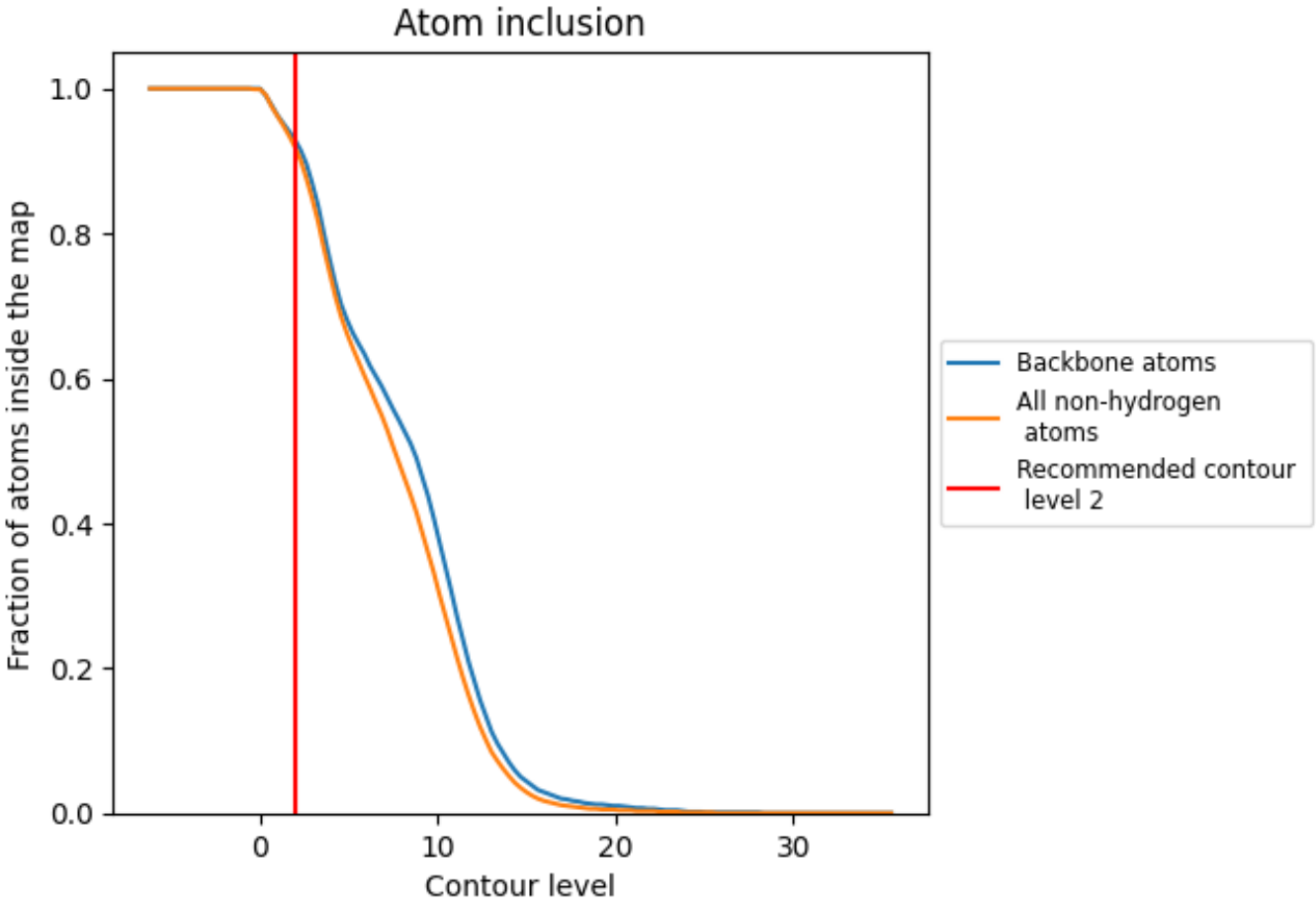
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.4360
A	0.9830	0.6320
B	0.9780	0.6240
C	0.9860	0.6420
D	0.9660	0.6150
E	0.9700	0.6100
F	1.0000	0.6580
G	0.9630	0.6320
H	0.9920	0.6480
I	0.9980	0.6070
J	0.9950	0.6010
K	0.9480	0.4960
L	0.1040	0.0440
M	0.8510	0.0780
N	0.9420	0.0810
O	0.2460	0.0660

